

## Author Index to Volume 159

- Ågren, H., S. Knuts, K.V. Mikkelsen and H.J.Aa. Jensen, Solvatochromatic shifts studied by multi-configuration self-consistent reaction field theory. Application to azabenzenes 159 (1992) 211
- Banjavčić, M.P., see T. Daniels 159 (1992) 289
- Benderskii, V.A., V.I. Goldanskii and D.E. Makarov, Two-dimensional trajectories of tunneling in the symmetric double-well potential 159 (1992) 29
- Bersuker, I.B., see V.Z. Polinger 159 (1992) 75
- Biggs, P., see J. Wildt 159 (1992) 127
- Billing, G.D., Quantum-classical reaction path model for chemical reactions. IV. The reaction  $\text{Cl}^- + \text{CH}_3\text{Cl} \rightarrow \text{ClCH}_3 + \text{Cl}^-$  159 (1992) 109
- Blaise, P., M. Giry and O. Henri-Rousseau, Driven damped harmonic oscillators perturbed by the parity operator 159 (1992) 169
- Bosch, E., M. Moreno and J.M. Lluch, A semiclassical simulation for tunneling dynamics of malonaldehyde and hydrogenoxalate anion 159 (1992) 99
- Brion, C.E., see P. Duffy 159 (1992) 347
- Brosolo, M. and P. Decleva, Variational approach to continuum orbitals in a spline basis: an application to  $\text{H}_2^+$  photoionization 159 (1992) 185
- Casarin, M., G. Granozzi, E. Tondello and A. Vittadini, A theoretical investigation of the electronic structure, hyperfine properties and binding energies of muonium centres in cuprous chloride 159 (1992) 365
- Casida, M.E., see P. Duffy 159 (1992) 347
- Chakraborty, T. and M. Chowdhury, Fluorescence excitation spectrum of 1,8-disubstituted naphthalenes in supersonic jet 159 (1992) 439
- Chapuisat, X., see C. Saint-Espès 159 (1992) 377
- Chapuisat, X. and C. Saint-Espès, A weak-mode representation of floppy molecules. II. Kinetic energy and total Hamiltonian matrix 159 (1992) 391
- Charutz, D.M. and R.D. Levine, The dynamics of dressed variables 159 (1992) 321
- Chong, D.P., see P. Duffy 159 (1992) 347
- Chowdhury, M., see T. Chakraborty 159 (1992) 439
- Cossart-Magos, C., see F. Morlet-Savary 159 (1992) 303
- Cuadros, F. and A. Mulero, The radial distribution function for two-dimensional Lennard-Jones fluids: computer simulation results 159 (1992) 89
- Cukrowski, A.S., A.L. Kawczyński, J. Popielawski, W. Stiller and R. Schmidt, Interaction between two chemical reactions in gases. The nonequilibrium effects from the Boltzmann and Fokker-Planck equations within a Lorentz gas model 159 (1992) 39
- Daniels, T., H. Zhu, M.P. Banjavčić and K.T. Leung, Valence-shell electron momentum distributions and ionization energy spectra of tetramethylsilane by symmetric noncoplanar (e, 2e) spectroscopy 159 (1992) 289
- Decleva, P., see M. Brosolo 159 (1992) 185

- Dimicoli, I., see F. Morlet-Savary 159 (1992) 303
- Duffy, P., M.E. Casida, C.E. Brion and D.P. Chong, Assessment of Gaussian-weighted angular resolution functions in the comparison of quantum-mechanically calculated electron momentum distributions with experiment 159 (1992) 347
- Farantos, S.C., The importance of periodic orbits in analysing photodissociation resonances: the  $O_3$  case 159 (1992) 329
- Fink, E.H., see J. Wildt 159 (1992) 127
- Gale, G.M., see P. Schanne 159 (1992) 1
- Giry, M., see P. Blaise 159 (1992) 169
- Goldanskii, V.I., see V.A. Benderskii 159 (1992) 29
- Gorinchoi, N.N., see V.Z. Polinger 159 (1992) 75
- Granozzi, G., see M. Casarin 159 (1992) 365
- Hald, M. and J.P. Jacobsen,  $^{23}Na$  relaxation in DNA solutions. Influence of intercalation on correlation times and coupling constants 159 (1992) 257
- Halvick, P., see M. Monnerville 159 (1992) 227
- Henri-Rousseau, O., see P. Blaise 159 (1992) 169
- Hermansson, K., From cluster to crystal: ab initio calculations of the  $OH^-$  frequency in lithium hydroxide monohydrate 159 (1992) 67
- Heyes, D.M., Chemical potential, partial enthalpy and partial volume of mixtures by *NPT* molecular dynamics 159 (1992) 149
- Holmlid, L., see E. Wallin 159 (1992) 313
- Jacobsen, J.P., see M. Hald 159 (1992) 257
- Jensen, H.J.Aa., see H. Ågren 159 (1992) 211
- Kawczyński, A.L., see A.S. Cukrowski 159 (1992) 39
- Kirski, T., see B. Stein 159 (1992) 269
- Klimo, V., J. Urban and J. Tiño, Quasiclassical trajectory study of the effect of reactant rotation on the reaction  $B^+ + HD \rightarrow BH^+ (BD^+) + D(H)$  159 (1992) 141
- Knuts, S., see H. Ågren 159 (1992) 211
- Kolenda, J., see B. Stein 159 (1992) 269
- Leung, K.T., see T. Daniels 159 (1992) 289
- Levine, R.D., see D.M. Charutz 159 (1992) 321
- Lluch, J.M., see E. Bosch 159 (1992) 99
- Makarov, D.E., see V.A. Benderskii 159 (1992) 29
- Mikkelsen, K.V., see H. Ågren 159 (1992) 211
- Moc, J., J.M. Rudziński and H. Ratajczak, Comparative study on the structures and energies of the  $SiX_3$ ,  $GeX_3$  and  $SnX_3$  series of radicals ( $X=H, F, Cl$ ) 159 (1992) 197
- Monnerville, M., P. Halvick and J.C. Rayez, Time-dependent calculation of the energy resolved state-to-state transition probabilities for three-atom exchange reactions 159 (1992) 227
- Moreno, M., see E. Bosch 159 (1992) 99

- Morlet-Savary, F., I. Dimicoli, C. Cossart-Magos and J.E. Parkin, Characterization of the  $\tilde{B}-\tilde{X}$  transition of the chlorobenzene cation prepared in non-equilibrium rotational population distributions by resonance enhanced multiphoton ionization 159 (1992) 303
- Moro, G.J., Master equation for site distributions describing barrier crossing in the presence of anisotropic diffusion 159 (1992) 421
- Mulero, A., see F. Cuadros 159 (1992) 89
- Nelander, B., A matrix isolation study of the water-formaldehyde complex. The far-infrared region 159 (1992) 281
- Parkin, J.E., see F. Morlet-Savary 159 (1992) 303
- Polinger, V.Z., N.N. Gorinchoi and I.B. Bersuker, MO LCAO analysis of the vibronic instability of the  $\text{CuCl}_3^-$  trigonal bipyramidal configuration. Critical view on the angular overlap model in vibronic problems 159 (1992) 75
- Popielawski, J., see A.S. Cukrowski 159 (1992) 39
- Ratajczak, H., see J. Moc 159 (1992) 197
- Rayez, J.C., see M. Monnerville 159 (1992) 227
- Rothamel, F., see B. Stein 159 (1992) 269
- Rudziński, J.M., see J. Moc 159 (1992) 197
- Saint-Espès, C., X. Chapuisat and F. Schneider, A weak-mode representation of floppy molecules. I. Potential energy 159 (1992) 377
- Saint-Espès, C., see X. Chapuisat 159 (1992) 391
- Schanne, P. and G.M. Gale, Interference and Fermi-resonant two-vibron bound states 159 (1992) 1
- Schmidt, R., see A.S. Cukrowski 159 (1992) 39
- Schneider, F., see C. Saint-Espès 159 (1992) 377
- Schneider, W. and W. Thiel, Ab initio calculation of anharmonic force fields for the methyl, silyl, germyl, and stannyl halides 159 (1992) 49
- Schurath, U., see M. Winter 159 (1992) 235
- Schurath, U., see K. Seranski 159 (1992) 247
- Seranski, K., see M. Winter 159 (1992) 235
- Seranski, K., M. Winter and U. Schurath, Site-resolved vibronic spectra of matrix-isolated NBr: comparison with model calculations 159 (1992) 247
- Snider, N., Energy transfer distributions for classical, collinear atom-diatom collisions 159 (1992) 339
- Stein, B., F. Rothamel, T. Kirski, J. Kolenda and C. von Borczyskowski, Optical and ODMR spectroscopy of an induced triplet X-trap in 1,4-dibromobenzene single crystals 159 (1992) 269
- Stiller, W., see A.S. Cukrowski 159 (1992) 39
- Thiel, W., see W. Schneider 159 (1992) 49
- Tiño, J., see V. Klimo 159 (1992) 141
- Tondello, E., see M. Casarin 159 (1992) 365
- Urban, J., see V. Klimo 159 (1992) 141
- Vilesov, A.F., see J. Wildt 159 (1992) 127
- Vittadini, A., see M. Casarin 159 (1992) 365

- Von Borczyskowski, C., see B. Stein 159 (1992) 269  
Von Niessen, W., see W. Wardermann 159 (1992) 11
- Wallin, E. and L. Holmlid, Excited states of hydrogen emitted from a graphite diffusion source: Arrhenius behaviour 159 (1992) 313
- Wardermann, W. and W. von Niessen, Satellite lines at the ionization threshold in charge transfer systems 159 (1992) 11
- Wayne, R.P., see J. Wildt 159 (1992) 127
- Wildt, J., E.H. Fink, P. Biggs, R.P. Wayne and A.F. Vilesov, Collision-induced emission of  $O_2(a^1\Delta_g \rightarrow X^3\Sigma_g^-)$  in the gas phase 159 (1992) 127
- Winter, M., K. Seranski and U. Schurath, Site effects in spectra of matrix-isolated diatomic molecules: a modelling approach 159 (1992) 235
- Winter, M., see K. Seranski 159 (1992) 247
- Zhu, H., see T. Daniels 159 (1992) 289

# List of Subjects

## 1 Methods

### 1.1 Theoretical

- 1.1.1 Group theory and algebras
- 1.1.2 Classical mechanics \*
- 1.1.3 Quantized field theory
- 1.1.4 Many body and quasiparticle approaches \*
- 1.1.5 Coupling schemes and perturbative treatments \*
- 1.1.6 Relativistic quantum mechanics
- 1.1.7 Transport quantum mechanics \*
- 1.1.8 Equilibrium statistical mechanics
- 1.1.9 Statistical mechanics of stationary states \*
- 1.1.10 Non-equilibrium thermodynamic and hydrodynamic theories \*
- 1.1.11 Ab initio schemes for stationary properties \*
- 1.1.12 Computational and simulation methods \*
- 1.1.13 Molecular dynamics and scattering theory \*

### 1.2 Experimental

- 1.2.1 Magnetic resonances \*
- 1.2.2 Cyclotron resonance
- 1.2.3 Microwave spectroscopy
- 1.2.4 Infrared spectroscopy \*
- 1.2.5 Raman spectroscopy
- 1.2.6 Visible and UV spectroscopy \*
- 1.2.7 Fluorescence spectroscopy \*
- 1.2.8 Photoelectron and Auger spectroscopy
- 1.2.9 X-ray spectroscopy
- 1.2.10 Electron impact spectroscopy \*
- 1.2.11 Laser methods \*
- 1.2.12 Picosecond spectroscopy
- 1.2.13 Non-linear optical spectroscopy
- 1.2.14 Synchrotron spectroscopies
- 1.2.15 Coherent optical spectroscopy
- 1.2.16 Optical pumping
- 1.2.17 Multiple resonance spectroscopy
- 1.2.18 Optoacoustic spectroscopy
- 1.2.19 Atomic and molecular beam techniques \*
- 1.2.20 Time-resolved experiments
- 1.2.21 Mass spectrometry \*
- 1.2.22 Radiolysis
- 1.2.23 Mössbauer spectroscopy
- 1.2.24 X-ray, electron and neutron diffraction
- 1.2.25 Neutron scattering
- 1.2.26 Light scattering
- 1.2.27 Field emission and field ionization \*
- 1.2.28 Measurement of macroscopic variables

## 2 Objects

### 2.1 Bulk systems

- 2.1.1 Gases \*
- 2.1.2 Supersonic beams \*
- 2.1.3 Liquids neat
- 2.1.4 Liquid mixtures and solutions \*
- 2.1.5 Crystals \*
- 2.1.5.1 neat \*
- 2.1.5.2 mixed \*
- 2.1.6 Glasses
- 2.1.7 Liquid crystals
- 2.1.8 Polymers
- 2.1.9 Semiconductors
- 2.1.10 Metals and alloys
- 2.1.11 Thin films
- 2.1.12 Surfaces
- 2.1.13 Low-dimensional materials \*
- 2.1.14 Dielectrics
- 2.1.15 Plasmas
- 2.1.16 Biological systems

### 2.2 Microscopic systems

- 2.2.1 Atoms \*
- 2.2.2 Molecules (neutral and ionic) \*
- 2.2.2.1 diatomic \*
- 2.2.2.2 small polyatomics \*
- 2.2.2.3 aromatics \*
- 2.2.2.4 other large
- 2.2.2.5 polymeric and biological \*
- 2.2.3 Molecular aggregates \*
- 2.2.3.1 dimers \*
- 2.2.3.2 van der Waals molecules
- 2.2.3.3 clusters \*
- 2.2.3.4 complexes \*
- 2.2.4 Free radicals (including hydronium and muonium) \*
- 2.2.5 Quasiparticles (including excitons)
- 2.2.6 Defects and impurities \*
- 2.2.7 Ions and charge carriers

\* Denotes subjects covered in this volume

### 3 Phenomena

- 3.1 Molecular structure \*
- 3.2 Vibrations and rotations of molecules \*
- 3.3 Electronic structure and states \*
- 3.4 Electric and magnetic properties \*
- 3.5 Spin splittings
- 3.6 Optical activity
- 3.7 Molecular interactions \*
- 3.8 Spectral bandshapes and intensities \*
- 3.9 Coupling of electronic and nuclear motion \*
- 3.10 Energy transfer processes \*
- 3.11 Molecular photophysical processes
- 3.12 Intramolecular dynamics \*
  - 3.12.1 radiationless transitions
  - 3.12.2 vibrational energy redistribution (including vibrational dissociation) \*
- 3.13 Luminescence spectra, yields and lifetimes \*
- 3.14 Coherence loss processes \*
- 3.15 Non-linear responses (including optical)
- 3.16 Multiphoton phenomena
- 3.17 Reactions (including dissociation) \*
  - 3.17.1 gas phase \*
  - 3.17.2 condensed phase \*
  - 3.17.3 photochemical
- 3.18 Tunnelling \*
- 3.19 Electron transfer
- 3.20 Positron annihilation
- 3.21 Ionization (including Rydberg states) \*
- 3.22 Molecular motion (including diffusive) \*
- 3.23 Isotopic effects
- 3.24 Fluctuations and noise
- 3.25 Collective motion and excitations
- 3.26 Surface effects and catalysis
- 3.27 Thermodynamic and transport properties \*
- 3.28 Structure of solids and liquids \*
- 3.29 Critical phenomena
- 3.30 Phase transitions

## Subject Index to Volume 159

### Methods

#### Theoretical

##### *Classical mechanics*

- Two-dimensional trajectories of tunneling in the symmetric double-well potential, V.A. Benderskii, V.I. Goldanskii and D.E. Makarov 159 (1992) 29
- Quasiclassical trajectory study of the effect of reactant rotation on the reaction  $B^+ + HD \rightarrow BH^+ (BD^+) + D(H)$ , V. Klimo, J. Urban and J. Tiño 159 (1992) 141
- The dynamics of dressed variables, D.M. Charutz and R.D. Levine 159 (1992) 321
- The importance of periodic orbits in analysing photodissociation resonances: the  $O_3$  case, S.C. Farantos 159 (1992) 329
- Energy transfer distributions for classical, collinear atom-diatom collisions, N. Snider 159 (1992) 339

##### *Many body and quasiparticle approaches*

- Interference and Fermi-resonant two-vibron bound states, P. Schanne and G.M. Gale 159 (1992) 1
- Satellite lines at the ionization threshold in charge transfer systems, W. Wardermann and W. von Niessen 159 (1992) 11
- Chemical potential, partial enthalpy and partial volume of mixtures by *NPT* molecular dynamics, D.M. Heyes 159 (1992) 149
- The dynamics of dressed variables, D.M. Charutz and R.D. Levine 159 (1992) 321

##### *Coupling schemes and perturbative treatments*

- Driven damped harmonic oscillators perturbed by the parity operator, P. Blaise, M. Giry and O. Henri-Rousseau 159 (1992) 169

##### *Transport quantum mechanics*

- Two-dimensional trajectories of tunneling in the symmetric double-well potential, V.A. Benderskii, V.I. Goldanskii and D.E. Makarov 159 (1992) 29

##### *Statistical mechanics of stationary states*

- Interaction between two chemical reactions in gases. The nonequilibrium effects from the Boltzmann and Fokker-Planck equations within a Lorentz gas model, A.S. Cukrowski, A.L. Kawczyński, J. Popielawski, W. Stiller and R. Schmidt 159 (1992) 39
- Chemical potential, partial enthalpy and partial volume of mixtures by *NPT* molecular dynamics, D.M. Heyes 159 (1992) 149

##### *Non-equilibrium thermodynamic and hydrodynamic theories*

- Driven damped harmonic oscillators perturbed by the parity operator, P. Blaise, M. Giry and O. Henri-Rousseau 159 (1992) 169

*Ab initio schemes for stationary properties*

- Ab initio calculation of anharmonic force fields for the methyl, silyl, germyl, and stannyl halides, W. Schneider and W. Thiel 159 (1992) 49
- From cluster to crystal: ab initio calculations of the OH<sup>-</sup> frequency in lithium hydroxide monohydrate, K. Hermansson 159 (1992) 67
- Variational approach to continuum orbitals in a spline basis: an application to H<sub>2</sub><sup>+</sup> photoionization, M. Brosolo and P. Decleva 159 (1992) 185
- Comparative study on the structures and energies of the SiX<sub>3</sub>, GeX<sub>3</sub> and SnX<sub>3</sub> series of radicals (X=H, F, Cl), J. Moc, J.M. Rudziński and H. Ratajczak 159 (1992) 197
- Solvatochromatic shifts studied by multi-configuration self-consistent reaction field theory. Application to azabenzenes, H. Ågren, S. Knuts, K.V. Mikkelsen and H.J.Aa. Jensen 159 (1992) 211

*Computational and simulation methods*

- MO LCAO analysis of the vibronic instability of the CuCl<sub>3</sub><sup>-</sup> trigonal bipyramidal configuration. Critical view on the angular overlap model in vibronic problems, V.Z. Polinger, N.N. Gorinchoi and I.B. Bersuker 159 (1992) 75
- The radial distribution function for two-dimensional Lennard-Jones fluids: computer simulation results, F. Cuadros and A. Mulero 159 (1992) 89
- A semiclassical simulation for tunneling dynamics of malonaldehyde and hydrogenoxalate anion, E. Bosch, M. Moreno and J.M. Lluch 159 (1992) 99
- Quasiclassical trajectory study of the effect of reactant rotation on the reaction B<sup>+</sup> + HD → BH<sup>+</sup> (BD<sup>+</sup>) + D(H), V. Klimo, J. Urban and J. Tiño 159 (1992) 141
- Chemical potential, partial enthalpy and partial volume of mixtures by NPT molecular dynamics, D.M. Heyes 159 (1992) 149
- Site effects in spectra of matrix-isolated diatomic molecules: a modelling approach, M. Winter, K. Seranski and U. Schurath 159 (1992) 235
- The dynamics of dressed variables, D.M. Charutz and R.D. Levine 159 (1992) 321
- Assessment of Gaussian-weighted angular resolution functions in the comparison of quantum-mechanically calculated electron momentum distributions with experiment, P. Duffy, M.E. Casida, C.E. Brion and D.P. Chong 159 (1992) 347
- A theoretical investigation of the electronic structure, hyperfine properties and binding energies of muonium centres in cuprous chloride, M. Casarin, G. Granozzi, E. Tondello and A. Vittadini 159 (1992) 365

*Molecular dynamics and scattering theory*

- The radial distribution function for two-dimensional Lennard-Jones fluids: computer simulation results, F. Cuadros and A. Mulero 159 (1992) 89
- A semiclassical simulation for tunneling dynamics of malonaldehyde and hydrogenoxalate anion, E. Bosch, M. Moreno and J.M. Lluch 159 (1992) 99
- Quantum-classical reaction path model for chemical reactions. IV. The reaction Cl<sup>-</sup> + CH<sub>3</sub>Cl → ClCH<sub>3</sub> + Cl<sup>-</sup>, G.D. Billing 159 (1992) 109
- Quasiclassical trajectory study of the effect of reactant rotation on the reaction B<sup>+</sup> + HD → BH<sup>+</sup> (BD<sup>+</sup>) + D(H), V. Klimo, J. Urban and J. Tiño 159 (1992) 141
- Variational approach to continuum orbitals in a spline basis: an application to H<sub>2</sub><sup>+</sup> photoionization, M. Brosolo and P. Decleva 159 (1992) 185
- Time-dependent calculation of the energy resolved state-to-state transition probabilities for three-atom exchange reactions, M. Monnerville, P. Halvick and J.C. Rayez 159 (1992) 227



- The importance of periodic orbits in analysing photodissociation resonances: the  $O_3$  case, S.C. Farantos 159 (1992) 329
- Energy transfer distributions for classical, collinear atom-diatom collisions, N. Snider 159 (1992) 339
- A weak-mode representation of floppy molecules. I. Potential energy, C. Saint-Espès, X. Chapuisat and F. Schneider 159 (1992) 377
- A weak-mode representation of floppy molecules. II. Kinetic energy and total Hamiltonian matrix, X. Chapuisat and C. Saint-Espès 159 (1992) 391
- Master equation for site distributions describing barrier crossing in the presence of anisotropic diffusion, G.J. Moro 159 (1992) 421

## Experimental

### Magnetic resonances

- $^{23}Na$  relaxation in DNA solutions. Influence of intercalation on correlation times and coupling constants, M. Hald and J.P. Jacobsen 159 (1992) 257
- Optical and ODMR spectroscopy of an induced triplet X-trap in 1,4-dibromobenzene single crystals, B. Stein, F. Rothamel, T. Kirski, J. Kolenda and C. von Borczyskowski 159 (1992) 269

### Infrared spectroscopy

- Collision-induced emission of  $O_2(a^1\Delta_g \rightarrow X^3\Sigma_g^-)$  in the gas phase, J. Wildt, E.H. Fink, P. Biggs, R.P. Wayne and A.F. Vilesov 159 (1992) 127
- A matrix isolation study of the water-formaldehyde complex. The far-infrared region, B. Nelander 159 (1992) 281

### Visible and UV spectroscopy

- Collision-induced emission of  $O_2(a^1\Delta_g \rightarrow X^3\Sigma_g^-)$  in the gas phase, J. Wildt, E.H. Fink, P. Biggs, R.P. Wayne and A.F. Vilesov 159 (1992) 127

### Fluorescence spectroscopy

- Site-resolved vibronic spectra of matrix-isolated NBr: comparison with model calculations, K. Seranski, M. Winter and U. Schurath 159 (1992) 247
- Optical and ODMR spectroscopy of an induced triplet X-trap in 1,4-dibromobenzene single crystals, B. Stein, F. Rothamel, T. Kirski, J. Kolenda and C. von Borczyskowski 159 (1992) 269
- Fluorescence excitation spectrum of 1,8-disubstituted naphthalenes in supersonic jet, T. Chakraborty and M. Chowdhury 159 (1992) 439

### Electron impact spectroscopy

- Valence-shell electron momentum distributions and ionization energy spectra of tetramethylsilane by symmetric noncoplanar ( $e, 2e$ ) spectroscopy, T. Daniels, H. Zhu, M.P. Banjavčić and K.T. Leung 159 (1992) 289
- Assessment of Gaussian-weighted angular resolution functions in the comparison of quantum-mechanically calculated electron momentum distributions with experiment, P. Duffy, M.E. Casida, C.E. Brion and D.P. Chong 159 (1992) 347

### Laser methods

- Fluorescence excitation spectrum of 1,8-disubstituted naphthalenes in supersonic jet, T. Chakraborty and M. Chowdhury 159 (1992) 439

*Atomic and molecular beam techniques*

- Excited states of hydrogen emitted from a graphite diffusion source: Arrhenius behaviour,  
E. Wallin and L. Holmlid 159 (1992) 313

*Mass spectrometry*

- Characterization of the  $\tilde{B} \leftarrow \tilde{X}$  transition of the chlorobenzene cation prepared in non-equilibrium rotational population distributions by resonance enhanced multiphoton ionization, F. Morlet-Savary, I. Dimicoli, C. Cossart-Magos and J.E. Parkin 159 (1992) 303

*Field emission and field ionization*

- Excited states of hydrogen emitted from a graphite diffusion source: Arrhenius behaviour,  
E. Wallin and L. Holmlid 159 (1992) 313

**Objects****Bulk systems***Gases*

- Interaction between two chemical reactions in gases. The nonequilibrium effects from the Boltzmann and Fokker-Planck equations within a Lorentz gas model, A.S. Cukrowski, A.L. Kawczyński, J. Popielawski, W. Stiller and R. Schmidt 159 (1992) 39
- Characterization of the  $\tilde{B} \leftarrow \tilde{X}$  transition of the chlorobenzene cation prepared in non-equilibrium rotational population distributions by resonance enhanced multiphoton ionization, F. Morlet-Savary, I. Dimicoli, C. Cossart-Magos and J.E. Parkin 159 (1992) 303

*Supersonic beams*

- Fluorescence excitation spectrum of 1,8-disubstituted naphthalenes in supersonic jet,  
T. Chakraborty and M. Chowdhury 159 (1992) 439

*Liquid mixtures and solutions*

- Chemical potential, partial enthalpy and partial volume of mixtures by *NPT* molecular dynamics, D.M. Heyes 159 (1992) 149
- Solvatochromatic shifts studied by multi-configuration self-consistent reaction field theory. Application to azabenzenes, H. Ågren, S. Knuts, K.V. Mikkelsen and H.J.Aa. Jensen 159 (1992) 211
- $^{23}\text{Na}$  relaxation in DNA solutions. Influence of intercalation on correlation times and coupling constants, M. Hald and J.P. Jacobsen 159 (1992) 257

*Crystals*

- Two-dimensional trajectories of tunneling in the symmetric double-well potential,  
V.A. Benderskii, V.I. Goldanskii and D.E. Makarov 159 (1992) 29

*-neat*

- Interference and Fermi-resonant two-vibron bound states, P. Schanne and G.M. Gale 159 (1992) 1

*-mixed*

- Optical and ODMR spectroscopy of an induced triplet X-trap in 1,4-dibromobenzene single crystals, B. Stein, F. Rothamel, T. Kirski, J. Kolenda and C. von Borczyskowski 159 (1992) 269

*Low-dimensional materials*

- The radial distribution function for two-dimensional Lennard-Jones fluids: computer simulation results, F. Cuadros and A. Mulero 159 (1992) 89

**Microscopic systems***Atoms*

- Time-dependent calculation of the energy resolved state-to-state transition probabilities for three-atom exchange reactions, M. Monnerville, P. Halvick and J.C. Rayez 159 (1992) 227
- Assessment of Gaussian-weighted angular resolution functions in the comparison of quantum-mechanically calculated electron momentum distributions with experiment, P. Duffy, M.E. Casida, C.E. Brion and D.P. Chong 159 (1992) 347

*Molecules (neutral and ionic)*

- MO LCAO analysis of the vibronic instability of the  $\text{CuCl}_3^{2-}$  trigonal bipyramidal configuration. Critical view on the angular overlap model in vibronic problems, V.Z. Polinger, N.N. Gorinchoi and I.B. Bersuker 159 (1992) 75
- The radial distribution function for two-dimensional Lennard-Jones fluids: computer simulation results, F. Cuadros and A. Mulero 159 (1992) 89
- Variational approach to continuum orbitals in a spline basis: an application to  $\text{H}_2^+$  photoionization, M. Brosolo and P. Decleva 159 (1992) 185

*-diatomic*

- Collision-induced emission of  $\text{O}_2(a^1\Delta_g \rightarrow X^3\Sigma_g^-)$  in the gas phase, J. Wildt, E.H. Fink, P. Biggs, R.P. Wayne and A.F. Vilesov 159 (1992) 127
- Quasiclassical trajectory study of the effect of reactant rotation on the reaction  $\text{B}^+ + \text{HD} \rightarrow \text{BH}^+ (\text{BD}^+) + \text{D}(\text{H})$ , V. Klimo, J. Urban and J. Tiño 159 (1992) 141
- Time-dependent calculation of the energy resolved state-to-state transition probabilities for three-atom exchange reactions, M. Monnerville, P. Halvick and J.C. Rayez 159 (1992) 227
- Site effects in spectra of matrix-isolated diatomic molecules: a modelling approach, M. Winter, K. Seranski and U. Schurath 159 (1992) 235
- Site-resolved vibronic spectra of matrix-isolated NBr: comparison with model calculations, K. Seranski, M. Winter and U. Schurath 159 (1992) 247
- Excited states of hydrogen emitted from a graphite diffusion source: Arrhenius behaviour, E. Wallin and L. Holmlid 159 (1992) 313

*-small polyatomics*

- Ab initio calculation of anharmonic force fields for the methyl, silyl, germyl, and stannyl halides, W. Schneider and W. Thiel 159 (1992) 49
- A semiclassical simulation for tunneling dynamics of malonaldehyde and hydrogenoxalate anion, E. Bosch, M. Moreno and J.M. Lluh 159 (1992) 99
- Quantum-classical reaction path model for chemical reactions. IV. The reaction  $\text{Cl}^- + \text{CH}_3\text{Cl} \rightarrow \text{ClCH}_3 + \text{Cl}^-$ , G.D. Billing 159 (1992) 109
- Valence-shell electron momentum distributions and ionization energy spectra of tetramethylsilane by symmetric noncoplanar (e, 2e) spectroscopy, T. Daniels, H. Zhu, M.P. Banjavčić and K.T. Leung 159 (1992) 289

- The importance of periodic orbits in analysing photodissociation resonances: the  $O_3$  case, S.C. Farantos 159 (1992) 329
- Assessment of Gaussian-weighted angular resolution functions in the comparison of quantum-mechanically calculated electron momentum distributions with experiment, P. Duffy, M.E. Casida, C.E. Brion and D.P. Chong 159 (1992) 347
- A weak-mode representation of floppy molecules. I. Potential energy, C. Saint-Espès, X. Chapuisat and F. Schneider 159 (1992) 377
- A weak-mode representation of floppy molecules. II. Kinetic energy and total Hamiltonian matrix, X. Chapuisat and C. Saint-Espès 159 (1992) 391
- aromatics*
- Satellite lines at the ionization threshold in charge transfer systems, W. Wardermann and W. von Niessen 159 (1992) 11
- Characterization of the  $\tilde{B} \leftarrow \tilde{X}$  transition of the chlorobenzene cation prepared in non-equilibrium rotational population distributions by resonance enhanced multiphoton ionization, F. Morlet-Savary, I. Dimicoli, C. Cossart-Magos and J.E. Parkin 159 (1992) 303
- Fluorescence excitation spectrum of 1,8-disubstituted naphthalenes in supersonic jet, T. Chakraborty and M. Chowdhury 159 (1992) 439
- polymeric and biological*
- $^{23}\text{Na}$  relaxation in DNA solutions. Influence of intercalation on correlation times and coupling constants, M. Hald and J.P. Jacobsen 159 (1992) 257
- Molecular aggregates*
- dimers*
- Driven damped harmonic oscillators perturbed by the parity operator, P. Blaise, M. Giry and O. Henri-Rousseau 159 (1992) 169
- clusters*
- From cluster to crystal: ab initio calculations of the  $\text{OH}^-$  frequency in lithium hydroxide monohydrate, K. Hermansson 159 (1992) 67
- complexes*
- MO LCAO analysis of the vibronic instability of the  $\text{CuCl}_3^{3-}$  trigonal bipyramidal configuration. Critical view on the angular overlap model in vibronic problems, V.Z. Polinger, N.N. Gorinchoi and I.B. Bersuker 159 (1992) 75
- Collision-induced emission of  $\text{O}_2(a^1\Delta_g \rightarrow X^3\Sigma_g^-)$  in the gas phase, J. Wildt, E.H. Fink, P. Biggs, R.P. Wayne and A.F. Vilesov 159 (1992) 127
- A matrix isolation study of the water-formaldehyde complex. The far-infrared region, B. Nelander 159 (1992) 281
- Free radicals (including hydronium and muonium)*
- Excited states of hydrogen emitted from a graphite diffusion source: Arrhenius behaviour, E. Wallin and L. Holmlid 159 (1992) 313

*Defects and impurities*

- Site effects in spectra of matrix-isolated diatomic molecules: a modelling approach, M. Winter, K. Seranski and U. Schurath 159 (1992) 235
- Site-resolved vibronic spectra of matrix-isolated NBr: comparison with model calculations, K. Seranski, M. Winter and U. Schurath 159 (1992) 247

**Phenomena***Molecular structure*

- MO LCAO analysis of the vibronic instability of the  $\text{CuCl}_3^{2-}$  trigonal bipyramidal configuration. Critical view on the angular overlap model in vibronic problems, V.Z. Polinger, N.N. Gorinchoi and I.B. Bersuker 159 (1992) 75
- Variational approach to continuum orbitals in a spline basis: an application to  $\text{H}_2^+$  photoionization, M. Brosolo and P. Decleva 159 (1992) 185
- Comparative study on the structures and energies of the  $\text{SiX}_3$ ,  $\text{GeX}_3$  and  $\text{SnX}_3$  series of radicals ( $\text{X}=\text{H}, \text{F}, \text{Cl}$ ), J. Moc, J.M. Rudziński and H. Ratajczak 159 (1992) 197
- A theoretical investigation of the electronic structure, hyperfine properties and binding energies of muonium centres in cuprous chloride, M. Casarin, G. Granozzi, E. Tondello and A. Vittadini 159 (1992) 365

*Vibrations and rotations of molecules*

- Interference and Fermi-resonant two-vibron bound states, P. Schanne and G.M. Gale 159 (1992) 1
- Ab initio calculation of anharmonic force fields for the methyl, silyl, germyl, and stannyl halides, W. Schneider and W. Thiel 159 (1992) 49
- From cluster to crystal: ab initio calculations of the  $\text{OH}^-$  frequency in lithium hydroxide monohydrate, K. Hermansson 159 (1992) 67
- Quasiclassical trajectory study of the effect of reactant rotation on the reaction  $\text{B}^+ + \text{HD} \rightarrow \text{BH}^+ (\text{BD}^+) + \text{D}(\text{H})$ , V. Klimo, J. Urban and J. Tiño 159 (1992) 141
- A matrix isolation study of the water-formaldehyde complex. The far-infrared region, B. Nelander 159 (1992) 281
- The importance of periodic orbits in analysing photodissociation resonances: the  $\text{O}_3$  case, S.C. Farantos 159 (1992) 329
- A weak-mode representation of floppy molecules. I. Potential energy, C. Saint-Espès, X. Chapuisat and F. Schneider 159 (1992) 377
- A weak-mode representation of floppy molecules. II. Kinetic energy and total Hamiltonian matrix, X. Chapuisat and C. Saint-Espès 159 (1992) 391

*Electronic structure and states*

- Satellite lines at the ionization threshold in charge transfer systems, W. Wardermann and W. von Niessen 159 (1992) 11
- Site-resolved vibronic spectra of matrix-isolated NBr: comparison with model calculations, K. Seranski, M. Winter and U. Schurath 159 (1992) 247
- Valence-shell electron momentum distributions and ionization energy spectra of tetramethylsilane by symmetric noncoplanar ( $e$ ,  $2e$ ) spectroscopy, T. Daniels, H. Zhu, M.P. Banjavčić and K.T. Leung 159 (1992) 289
- Assessment of Gaussian-weighted angular resolution functions in the comparison of quantum-mechanically calculated electron momentum distributions with experiment, P. Duffy, M.E. Casida, C.E. Brion and D.P. Chong 159 (1992) 347

- A theoretical investigation of the electronic structure, hyperfine properties and binding energies of muonium centres in cuprous chloride, M. Casarin, G. Granozzi, E. Tondello and A. Vittadini 159 (1992) 365
- Electric and magnetic properties*
- $^{23}\text{Na}$  relaxation in DNA solutions. Influence of intercalation on correlation times and coupling constants, M. Hald and J.P. Jacobsen 159 (1992) 257
- Molecular interactions*
- Collision-induced emission of  $\text{O}_2(a^1\Delta_g \rightarrow X^3\Sigma_g^-)$  in the gas phase, J. Wildt, E.H. Fink, P. Biggs, R.P. Wayne and A.F. Vilesov 159 (1992) 127
- Site effects in spectra of matrix-isolated diatomic molecules: a modelling approach, M. Winter, K. Seranski and U. Schurath 159 (1992) 235
- A matrix isolation study of the water-formaldehyde complex. The far-infrared region, B. Nelander 159 (1992) 281
- Spectral bandshapes and intensities*
- Driven damped harmonic oscillators perturbed by the parity operator, P. Blaise, M. Giry and O. Henri-Rousseau 159 (1992) 169
- Characterization of the  $\tilde{B}-\tilde{X}$  transition of the chlorobenzene cation prepared in non-equilibrium rotational population distributions by resonance enhanced multiphoton ionization, F. Morlet-Savary, I. Dimicoli, C. Cossart-Magos and J.E. Parkin 159 (1992) 303
- Coupling of electronic and nuclear motion*
- MO LCAO analysis of the vibronic instability of the  $\text{CuCl}_3^{2-}$  trigonal bipyramidal configuration. Critical view on the angular overlap model in vibronic problems, V.Z. Polinger, N.N. Gorinchoi and I.B. Bersuker 159 (1992) 75
- Fluorescence excitation spectrum of 1,8-disubstituted naphthalenes in supersonic jet, T. Chakraborty and M. Chowdhury 159 (1992) 439
- Energy transfer processes*
- Optical and ODMR spectroscopy of an induced triplet X-trap in 1,4-dibromobenzene single crystals, B. Stein, F. Rothamel, T. Kirski, J. Kolenda and C. von Borczyskowski 159 (1992) 269
- Energy transfer distributions for classical, collinear atom-diatom collisions, N. Snider 159 (1992) 339
- Intramolecular dynamics*
- From cluster to crystal: ab initio calculations of the  $\text{OH}^-$  frequency in lithium hydroxide monohydrate, K. Hermansson 159 (1992) 67
- A semiclassical simulation for tunneling dynamics of malonaldehyde and hydrogenoxalate anion, E. Bosch, M. Moreno and J.M. Lluch 159 (1992) 99
- The dynamics of dressed variables, D.M. Charutz and R.D. Levine 159 (1992) 321
- A weak-mode representation of floppy molecules. I. Potential energy, C. Saint-Espès, X. Chapuisat and F. Schneider 159 (1992) 377
- A weak-mode representation of floppy molecules. II. Kinetic energy and total Hamiltonian matrix, X. Chapuisat and C. Saint-Espès 159 (1992) 391



*-vibrational energy redistribution (including vibrational dissociation)*

- Driven damped harmonic oscillators perturbed by the parity operator, P. Blaise, M. Giry and O. Henri-Rousseau 159 (1992) 169
- The importance of periodic orbits in analysing photodissociation resonances: the O<sub>3</sub> case, S.C. Farantos 159 (1992) 329

*Luminescence spectra, yields and lifetimes*

- Solvatochromatic shifts studied by multi-configuration self-consistent reaction field theory. Application to azabenzenes, H. Ågren, S. Knuts, K.V. Mikkelsen and H.J.Aa. Jensen 159 (1992) 211

*Coherence loss processes*

- Optical and ODMR spectroscopy of an induced triplet X-trap in 1,4-dibromobenzene single crystals, B. Stein, F. Rothamel, T. Kirski, J. Kolenda and C. von Borczyskowski 159 (1992) 269

*Reactions (including dissociation)*

- Time-dependent calculation of the energy resolved state-to-state transition probabilities for three-atom exchange reactions, M. Monnerville, P. Halvick and J.C. Rayez 159 (1992) 227
- Master equation for site distributions describing barrier crossing in the presence of anisotropic diffusion, G.J. Moro 159 (1992) 421

*-gas phase*

- Interaction between two chemical reactions in gases. The nonequilibrium effects from the Boltzmann and Fokker-Planck equations within a Lorentz gas model, A.S. Cukrowski, A.L. Kawczyński, J. Popielawski, W. Stiller and R. Schmidt 159 (1992) 39
- Quantum-classical reaction path model for chemical reactions. IV. The reaction  $\text{Cl}^- + \text{CH}_3\text{Cl} \rightarrow \text{ClCH}_3 + \text{Cl}^-$ , G.D. Billing 159 (1992) 109

*-condensed phase*

- Two-dimensional trajectories of tunneling in the symmetric double-well potential, V.A. Benderskii, V.I. Goldanskii and D.E. Makarov 159 (1992) 29
- Site-resolved vibronic spectra of matrix-isolated NBr: comparison with model calculations, K. Seranski, M. Winter and U. Schurath 159 (1992) 247
- The dynamics of dressed variables, D.M. Charutz and R.D. Levine 159 (1992) 321

*Tunnelling*

- Two-dimensional trajectories of tunneling in the symmetric double-well potential, V.A. Benderskii, V.I. Goldanskii and D.E. Makarov 159 (1992) 29
- A semiclassical simulation for tunneling dynamics of malonaldehyde and hydrogenoxalate anion, E. Bosch, M. Moreno and J.M. Lluch 159 (1992) 99

*Ionization (including Rydberg states)*

- Satellite lines at the ionization threshold in charge transfer systems, W. Wardermann and W. von Niessen 159 (1992) 11
- Excited states of hydrogen emitted from a graphite diffusion source: Arrhenius behaviour, E. Wallin and L. Holmlid 159 (1992) 313

*Molecular motion (including diffusive)*

- Master equation for site distributions describing barrier crossing in the presence of anisotropic diffusion, G.J. Moro 159 (1992) 421

*Thermodynamic and transport properties*

- Chemical potential, partial enthalpy and partial volume of mixtures by *NPT* molecular dynamics, D.M. Heyes 159 (1992) 149

*Structure of solids and liquids*

- The radial distribution function for two-dimensional Lennard-Jones fluids: computer simulation results, F. Cuadros and A. Mulero 159 (1992) 89



